Algorithm for generating quasiperiodic packings of icosahedral three-shell clusters

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Introduction

The strip projection method is the most important way to generate quasiperiodic patterns with predefined local structure. We have obtained a very efficient algorithm for this method which allows one to use it in superspaces of very high dimension. A version of this algorithm for two-dimensional clusters and an application to decagonal two-shell clusters (strip projection in a 10-dimensional superspace) has been presented in math-ph/0504036. The program in FORTRAN 90 used in this case is very fast (700-800 points are obtained in 3 minutes).

We present an application of our algorithm to three-dimensional clusters. The physical three-dimensional space is embedded into a 31-dimensional superspace and the strip projection method is used in order to generate a quasiperiodic packing of interpenetrating translated copies of a three-shell icosahedral cluster formed by the 12 vertices of a regular icosahedron (the first shell), the 20 vertices of a regular dodecahedron (the second shell) and the 30 vertices of an icosidodecahedron (the third shell).

On a personal computer Pentium 4 with Fortran PowerStation version 4.0 (Microsoft Developer Studio) we obtain 400-500 points in 10 minutes.

More details, bibliography and samples can be found on the website:

http://fpcm5.fizica.unibuc.ro∼ncotfas/

Computer program in FORTRAN 90 and MATHEMATICA

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! QUASIPERIODIC PACKINGS OF THREE-SHELL ICOSAHEDRAL CLUSTERS
! *****(ICOSAHEDRON + DODECAHEDRON + ICOSIDODECAHEDRON)*****

! PLEASE INDICATE THE NUMBER OF POINTS YOU WANT TO ANALYSE
      INTEGER, PARAMETER :: N = 10000

! PLEASE INDICATE THE DIMENSION  M OF THE SUPERSPACE
      INTEGER, PARAMETER :: M = 31
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      INTEGER  I, J, K, L, I1, I2, I3, I4, JJ, JP, JPP
      REAL T, R1, R2, R3, D1, D2, D3, D4, AA
  REAL, DIMENSION(M) :: V, W, TR
  REAL, DIMENSION(3,3) :: C5
  REAL, DIMENSION(3,M) :: B
  REAL, DIMENSION(1:M-3,2:M-2,3:M-1,4:M) :: S
  REAL, DIMENSION(N,M) :: P
  REAL, DIMENSION(N) :: X, Y, Z

! PLEASE INDICATE THE RADIUS OF THE FIRST SHELL (ICOSAHEDRON)
  R1 = 1.0

! PLEASE INDICATE THE RADIUS OF THE SECOND SHELL (DODECAHEDRON)
  R2 = 1.2

 ! PLEASE INDICATE THE RADIUS OF THE THIRD SHELL (ICOSIDODECAHEDRON)
  R3 = 1.5

! PLEASE INDICATE THE TRANSLATION OF THE STRIP YOU WANT TO USE
  TR = 0.1

  T = (1+SQRT(5.0))/2.0
  C5(1,1) = (T-1)/2.0
  C5(1,2) = -T/2.0
  C5(1,3) = 1/2.0
  C5(2,1) = T/2.0
  C5(2,2) = 1/2.0
  C5(2,3) = (T-1)/2.0
  C5(3,1) = -1/2.0
  C5(3,2) = (T-1)/2.0
  C5(3,3) = T/2.0
  B = 0.0
  B(1,1) = R1 / SQRT(T+2.0)
  B(2,1) = T * R1 / SQRT(T+2.0)
  DO I = 2, 5
    DO J = 1, 3
B(J,I) = SUM( C5(J,:) * B(:,I-1))
END DO
  END DO
  B(2,6) = R1 / SQRT(T+2.0)
  B(3,6) = T * R1 / SQRT(T+2.0)
      B(1,7) = R2 / SQRT(3.0)
  B(2,7) = R2 / SQRT(3.0)
  B(3,7) = R2 / SQRT(3.0)
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  DO I = 8, 11
    DO J = 1, 3
B(J,I) = SUM( C5(J,:) * B(:,I-1))
END DO
  END DO
  B(1,12) = R2 / SQRT(3.0)
  B(2,12) = -R2 / SQRT(3.0)
  B(3,12) = R2 / SQRT(3.0)
  DO I = 13, 16
    DO J = 1, 3
B(J,I) = SUM( C5(J,:) * B(:,I-1))
END DO
  END DO
  B(1,17) = R3
  DO I = 18, 21
    DO J = 1, 3
B(J,I) = SUM( C5(J,:) * B(:,I-1))
END DO
  END DO
  B(2,22) = R3
  DO I = 23, 26
    DO J = 1, 3
B(J,I) = SUM( C5(J,:) * B(:,I-1))
END DO
  END DO
  B(3,27) = R3
  DO I = 28, 31
    DO J = 1, 3
B(J,I) = SUM( C5(J,:) * B(:,I-1))
END DO
  END DO
  PRINT*, 'RADIUS OF THE FIRST SHELL (ICOSAHEDRON) IS ', R1
  PRINT*, 'RADIUS OF THE SECOND SHELL (DODECAHEDRON) IS ', R2
  PRINT*, 'RADIUS OF THE THIRD SHELL (ICOSIDODECAHEDRON) IS ', R3
  PRINT*, 'STRIP TRANSLATED IN SUPERSPACE WITH THE VECTOR OF COORDINATES:'
  PRINT*, TR
  PRINT*, 'COORDINATES OF THE POINTS OF THREE-SHELL ICOSAHEDRAL CLUSTER'
  PRINT*, '  (UP TO A SYMMETRY WITH RESPECT TO THE ORIGIN):'
  DO J = 1, M
  PRINT*, J, B(1,J), B(2,J), B(3,J)
  END DO
  PRINT*, 'PLEASE WAIT A FEW MINUTES OR MORE,&
           DEPENDING ON THE NUMBER OF ANALYSED POINTS'

      S = 0
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      DO I1 = 1, M-3
      DO I2 = I1+1, M-2
      DO I3 = I2+1, M-1
      DO I4 = I3+1, M
    DO D1 = -0.5, 0.5
DO D2 = -0.5, 0.5
DO D3 = -0.5, 0.5
DO D4 = -0.5, 0.5
    AA = D1 * ( B(1,I2) * B(2,I3) * B(3,I4) + &
            B(2,I2) * B(3,I3) * B(1,I4) + &
B(3,I2) * B(1,I3) * B(2,I4) - &
B(3,I2) * B(2,I3) * B(1,I4) - &
            B(1,I2) * B(3,I3) * B(2,I4) - &
B(2,I2) * B(1,I3) * B(3,I4) ) - &
 D2 * ( B(1,I1) * B(2,I3) * B(3,I4) + &
            B(2,I1) * B(3,I3) * B(1,I4) + &
B(3,I1) * B(1,I3) * B(2,I4) - &
B(3,I1) * B(2,I3) * B(1,I4) - &
            B(1,I1) * B(3,I3) * B(2,I4) - &
B(2,I1) * B(1,I3) * B(3,I4) ) + &
 D3 * ( B(1,I1) * B(2,I2) * B(3,I4) + &
            B(2,I1) * B(3,I2) * B(1,I4) + &
B(3,I1) * B(1,I2) * B(2,I4) - &
B(3,I1) * B(2,I2) * B(1,I4) - &
            B(1,I1) * B(3,I2) * B(2,I4) - &
B(2,I1) * B(1,I2) * B(3,I4) ) - &
 D4 * ( B(1,I1) * B(2,I2) * B(3,I3) + &
            B(2,I1) * B(3,I2) * B(1,I3) + &
B(3,I1) * B(1,I2) * B(2,I3) - &
B(3,I1) * B(2,I2) * B(1,I3) - &
            B(1,I1) * B(3,I2) * B(2,I3) - &
B(2,I1) * B(1,I2) * B(3,I3) )
IF ( AA > S(I1,I2,I3,I4) )  S(I1,I2,I3,I4) = AA
   END DO
        END DO
        END DO
        END DO
   IF( S(I1,I2,I3,I4) == 0) S(I1,I2,I3,I4) = N * SUM( B(1,:) ** 2 )
  END DO
      END DO
      END DO
      END DO
      P = 0
  P( 1,:) = ANINT( TR )
  K = 1
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  L = 0
  JP = 0
  DO I = 1, N
  IF( I <= K ) THEN
  V = P(I, : ) - TR
  JJ = 1
  JPP = 0
    DO I1 = 1, M-3
        DO I2 = I1+1, M-2
        DO I3 = I2+1, M-1
        DO I4 = I3+1, M
    AA = V(I1) * ( B(1,I2) * B(2,I3) * B(3,I4) + &
               B(2,I2) * B(3,I3) * B(1,I4) + &
       B(3,I2) * B(1,I3) * B(2,I4) - &
   B(3,I2) * B(2,I3) * B(1,I4) - &
               B(1,I2) * B(3,I3) * B(2,I4) - &
   B(2,I2) * B(1,I3) * B(3,I4) ) - &
 V(I2) * ( B(1,I1) * B(2,I3) * B(3,I4) + &
               B(2,I1) * B(3,I3) * B(1,I4) + &
   B(3,I1) * B(1,I3) * B(2,I4) - &
   B(3,I1) * B(2,I3) * B(1,I4) - &
               B(1,I1) * B(3,I3) * B(2,I4) - &
   B(2,I1) * B(1,I3) * B(3,I4) ) + &
 V(I3) * ( B(1,I1) * B(2,I2) * B(3,I4) + &
               B(2,I1) * B(3,I2) * B(1,I4) + &
   B(3,I1) * B(1,I2) * B(2,I4) - &
   B(3,I1) * B(2,I2) * B(1,I4) - &
               B(1,I1) * B(3,I2) * B(2,I4) - &
   B(2,I1) * B(1,I2) * B(3,I4) ) - &
 V(I4) * ( B(1,I1) * B(2,I2) * B(3,I3) + &
               B(2,I1) * B(3,I2) * B(1,I3) + &
   B(3,I1) * B(1,I2) * B(2,I3) - &
   B(3,I1) * B(2,I2) * B(1,I3) - &
               B(1,I1) * B(3,I2) * B(2,I3) - &
   B(2,I1) * B(1,I2) * B(3,I3) )
IF ( AA < -S(I1,I2,I3,I4) .OR. AA > S(I1,I2,I3,I4) )  JJ = 0
IF ( AA == -S(I1,I2,I3,I4) .OR. AA == S(I1,I2,I3,I4) )  JPP = 1
END DO
        END DO
        END DO
        END DO

IF ( JJ .EQ. 1 ) THEN
XP =  SUM( V * B(1,:) )
    YP =  SUM( V * B(2,:) )
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ZP =  SUM( V * B(3,:) )
    I3 = 1
IF ( L > 0) THEN
       DO J = 1, L
       IF( XP == X(J) .AND. YP == Y(J) .AND. ZP == Z(J) ) I3 = 0
       END DO
ELSE
END IF
    IF( I3 == 1) THEN
    IF( JPP .EQ. 1 ) JP = JP + 1
        L = L + 1
X(L) = XP
        Y(L) = YP
Z(L) = ZP
ELSE
    END IF
DO I1 = 1, M
 DO I2 = -1, 1
  W = P(I,:)
  W(I1) = W(I1) + I2
  I3 = 0
   DO J = 1, K
   IF( ALL(W .EQ. P(J,:)) ) I3 = 1
           END DO
    IF( I3 == 0 .AND. K < N ) THEN
K = K + 1
P(K, : ) = W
ELSE
END IF
 END DO
END DO
ELSE
   END IF
  ELSE
  END IF
  END DO
  PRINT*, 'NUMBER OF ANALYSED POINTS : ', K
  PRINT*, 'NUMBER OF OBTAINED POINTS : ', L
      PRINT*, 'NUMBER OF POINTS LYING ON THE FRONTIERE OF THE &
                                                  STRIP:', JP
  PRINT*, 'PLEASE INDICATE THE NAME OF A FILE FOR RESULTS'
      WRITE(4,98)
  98  FORMAT('Show[Graphics3D[{ PointSize[0.01],{')
  DO J = 1, L-1
  WRITE(4,99) X(J), Y(J), Z(J)
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  99  FORMAT( 'Point[{'F10.5','F10.5','F10.5,'}], ')
  END DO
     WRITE(4,100) X(L), Y(L), Z(L)
 100  FORMAT( 'Point[{'F10.5','F10.5','F10.5,'}]')
  WRITE(4,101)
 101  FORMAT('}} ]]')
PRINT*, '* OPEN THE FILE CONTAINING THE RESULTS WITH &
                                                "NotePad" '
PRINT*, '* SELECT THE CONTENT OF THE FILE ("Select All") &
                                         AND COPY IT ("Copy")'
PRINT*, '* OPEN "MATHEMATICA", PASTE THE COPIED FILE, &
                               AND EXECUTE IT ("Shift+Enter")'

  END
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